Bren School of Environmental Science & Management
UNIVERSITY OF CALIFORNIA, SANTA BARBARA

Alternatives Analysis Workshop on Life Cycle Impacts & Exposure Assessment

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APPLICATION OF LIFE CYCLE AND EXPOSURE ASSESSMENT TOOLS TO ALTERNATIVES ANALYSIS

Dr. Sangwon Suh & Dr. Arturo Keller

APPLICATION OF LIFE CYCLE TOOLS TO ALTERNATIVES ANALYSIS

Dr. Sangwon Suh (Aug 9th, 3:00pm-3:30pm)

Outline

- Identification of relevant factors
- LCA resources
- Limitations of LCA approach to AA

Relevant Factors

Identify Relevant Factors

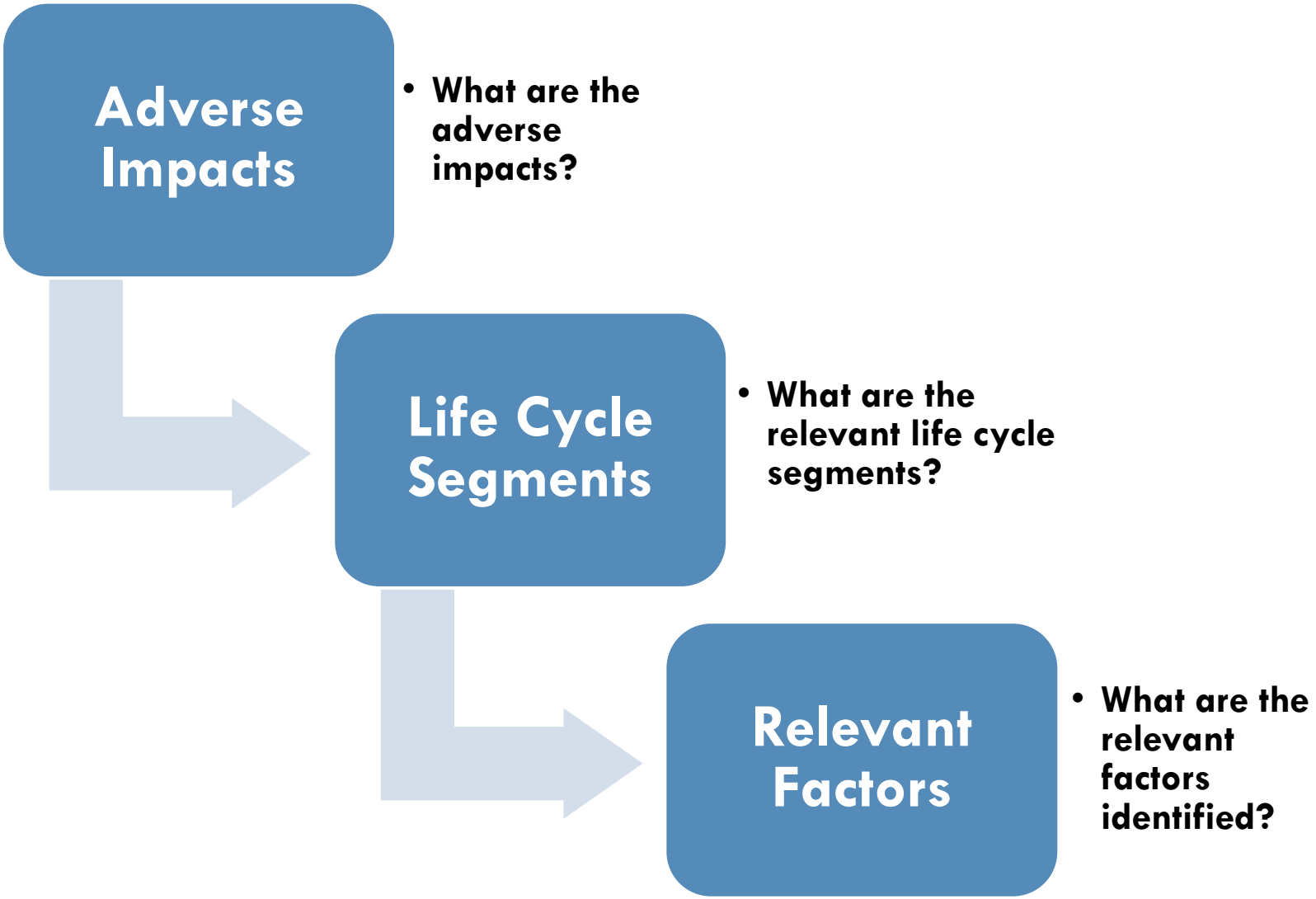


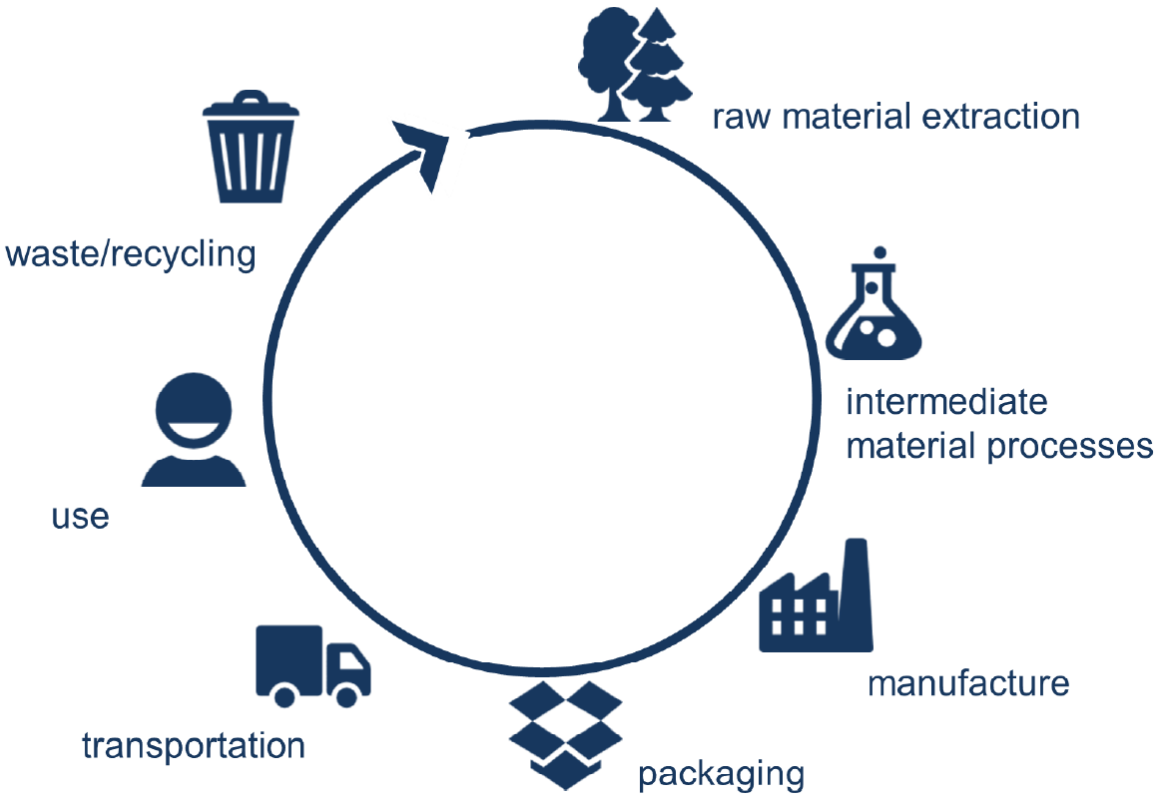
Table 5-1 Relevant Life Cycle Segments & Factors					
Relevant		Priority Product	ALT 1	ALT 2	ALT 3-10
Life Cycle Segment	Factors or Impacts				
Raw Material Extraction	Environmental Impacts	H	o	o	o
	Public Health Impacts	H	o	o	o
	Waste and End-of life				
	Environmental Fate	H	M	M	
	Materials & Resource Consumption Impacts				
	Physical chemical hazards				
	Physiochemical properties				
Intermediate Process	Environmental Impacts				
	Public Health Impacts				
	Waste and End-of life				
	Environmental Fate				
	Materials & Resource Consumption Impacts	M	H	L	H
	Physical chemical hazards				
	Physiochemical properties				
MFR	Environmental Impacts	H			
	Public Health Impacts	M			
	Waste and End-of life				
	Environmental Fate	H			
	Materials & Resource Consumption Impacts				
	Physical chemical hazards				
	Physiochemical properties				
Packaging & Transportation		⊘	⊘	⊘	⊘
Distribution		⊘	⊘	⊘	⊘
Use	Environmental Impacts	H	L	H	M
	Public Health Impacts	H	M	M	M
	Waste and End-of life				
	Environmental Fate	M	H	L	H
	Materials & Resource Consumption Impacts				
	Physical chemical hazards				
	Physiochemical properties				
Operation & Maintenance		⊘	⊘	⊘	⊘
Reuse & Recycling	Environmental Impacts	H	o	M	
	Public Health Impacts	L	o	L	
	Waste and End-of-life	H		M	
	Environmental Fate	H		M	
	Materials & Resource Consumption Impacts				
	Physical chemical hazards				
	Physiochemical properties				
End-of-Life		⊘	⊘	⊘	⊘

H = High Impact observed
M = Medium Impact observed
L = Low Impact observed
● - Data not available (impact not quantifiable)
o - Data not available
⊘ - Not Applicable

From AA Guide p59

Choose a chemical of your interest and answer the following questions.

Things to Consider

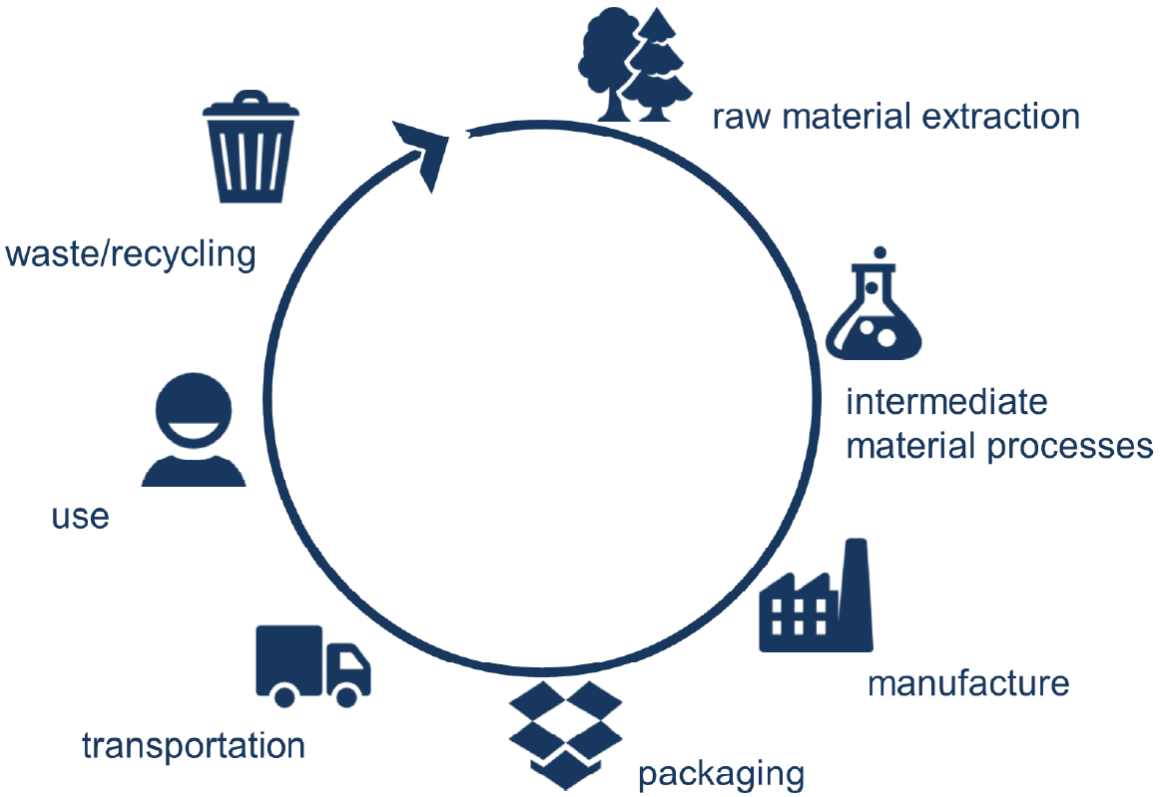


Raw Materials Extraction

- Are rare materials involved in the extraction?
- Is there a new risk introduced in the extraction process with the alternatives (e.g., use of explosives)?

From AA Guide p82

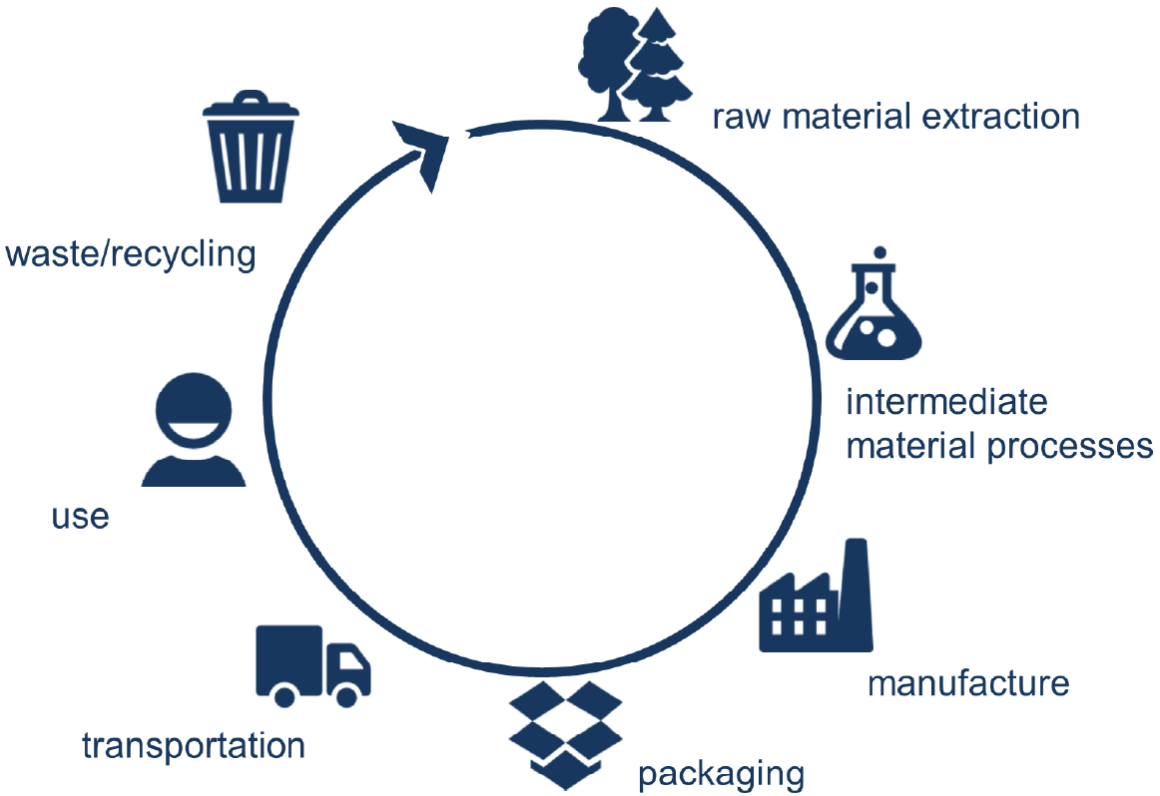
Things to Consider



Intermediate Materials Processes

- Are there any intermediate processes different? (e.g., refining, milling, spinning, etc.)

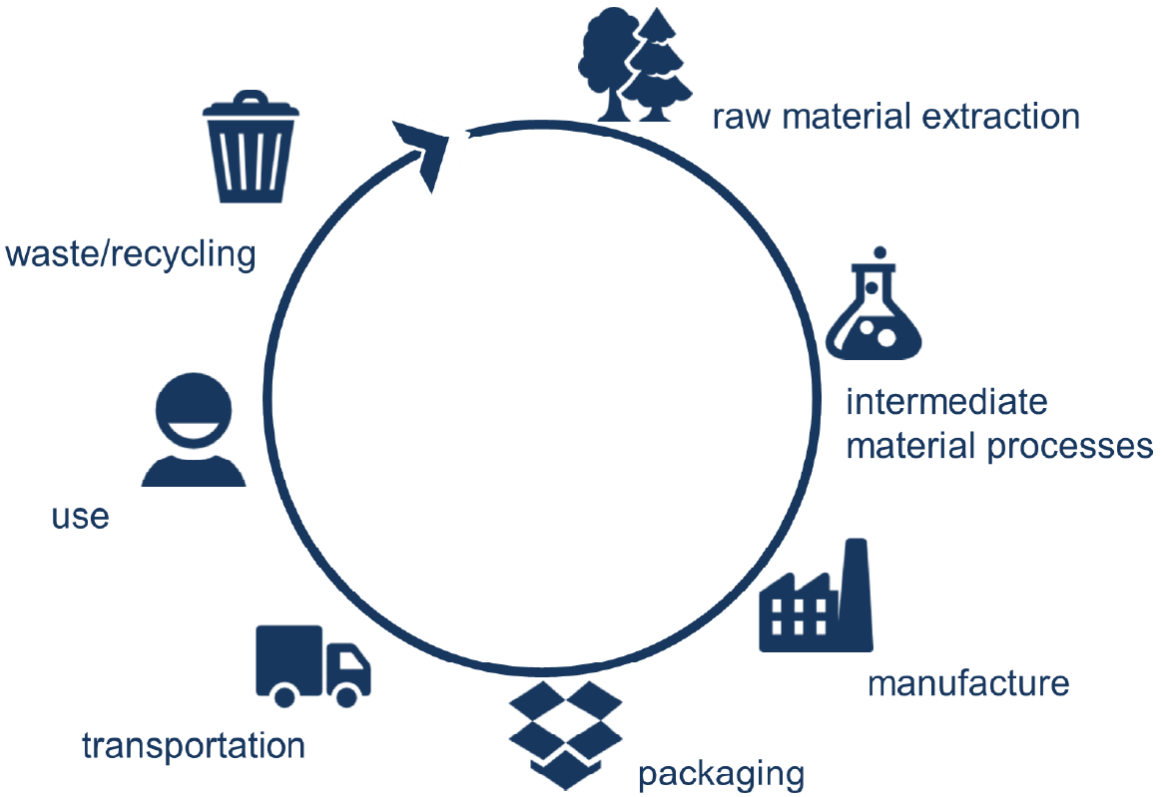
Things to Consider



Manufacturing (part 1)

- Are additional materials required to manufacture the alternatives?
- Will there be significant increases in the use of energy or water?
- Will there be additional air emissions or releases to water or soil?

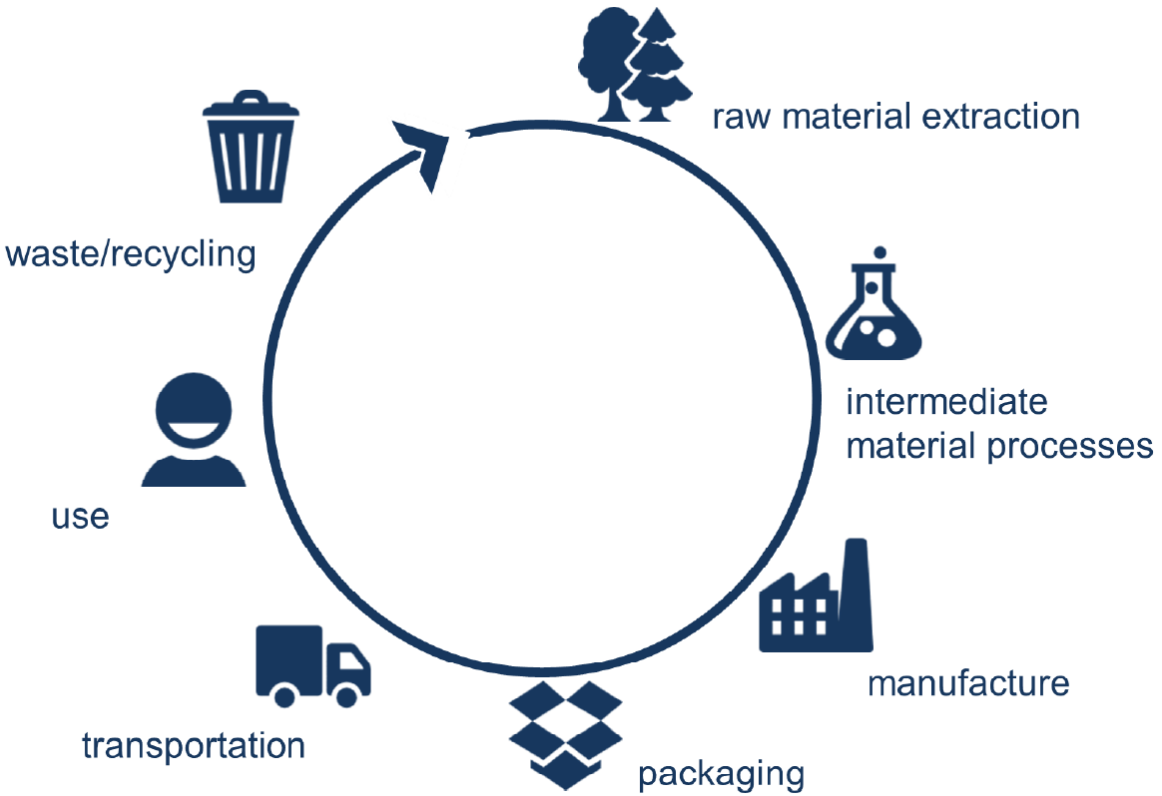
Things to Consider



Manufacturing (part 2)

- Will solid waste generation be increased due to the selection of an alternative?
- Were manufacturing worker exposures important as a basis for listing the Priority Product?

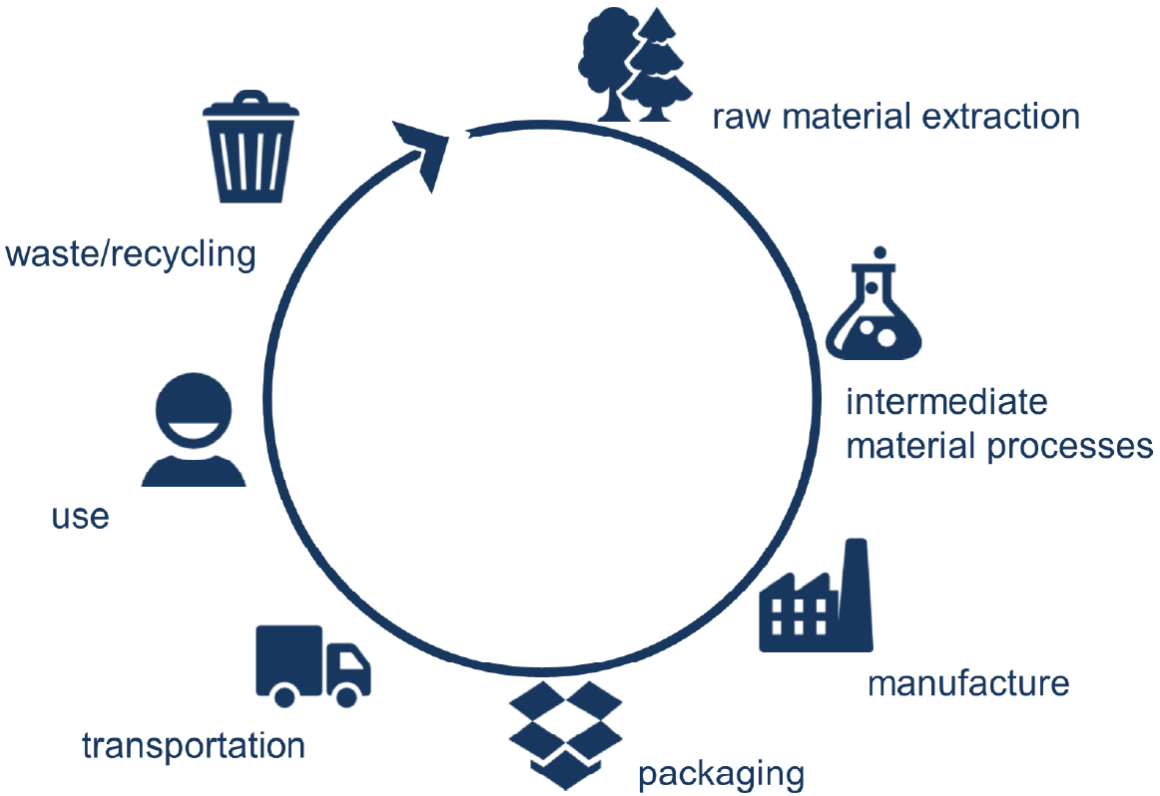
Things to Consider



Packaging

- Will there be differences in the type and quantity of materials used for packaging?
- Does the packaging need to be changed to be compatible with any of the alternatives under consideration?

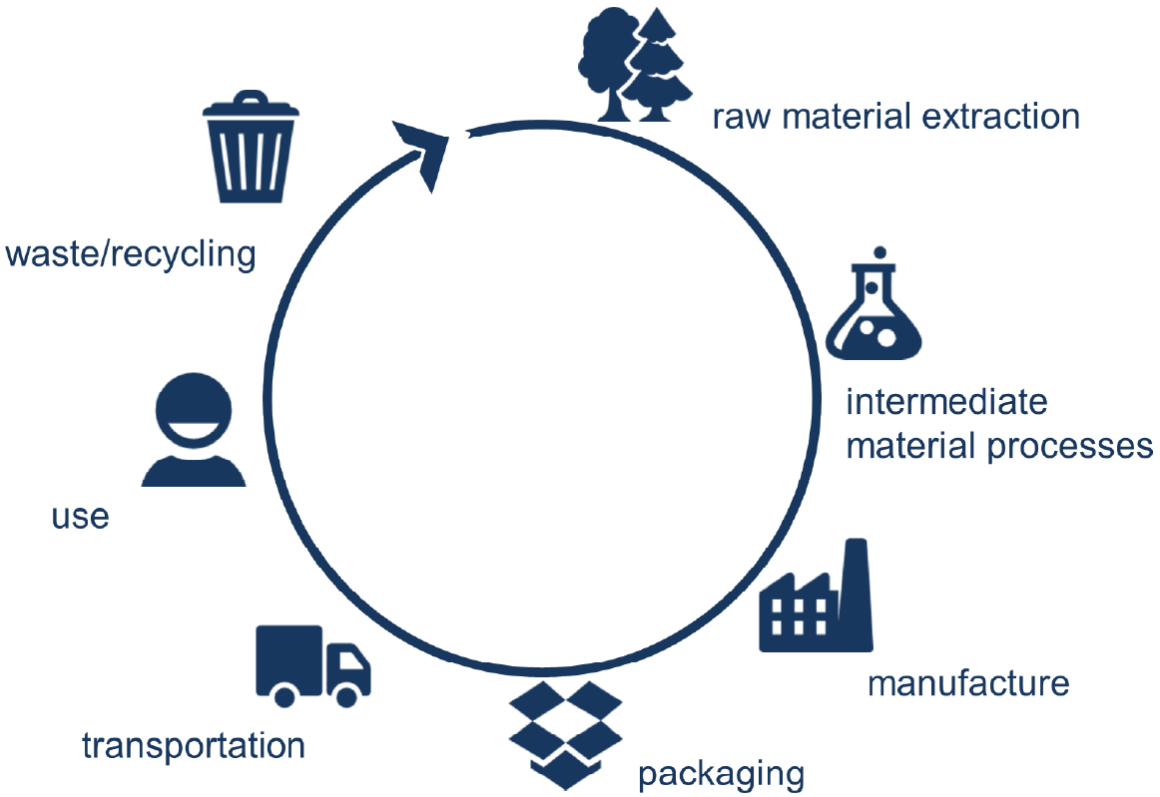
Things to Consider



Transportation

- Is a different mode of transport required for the alternatives?
- How far are the materials to be transported?
- Will there be an increase in greenhouse gases due to increased transportation distance?

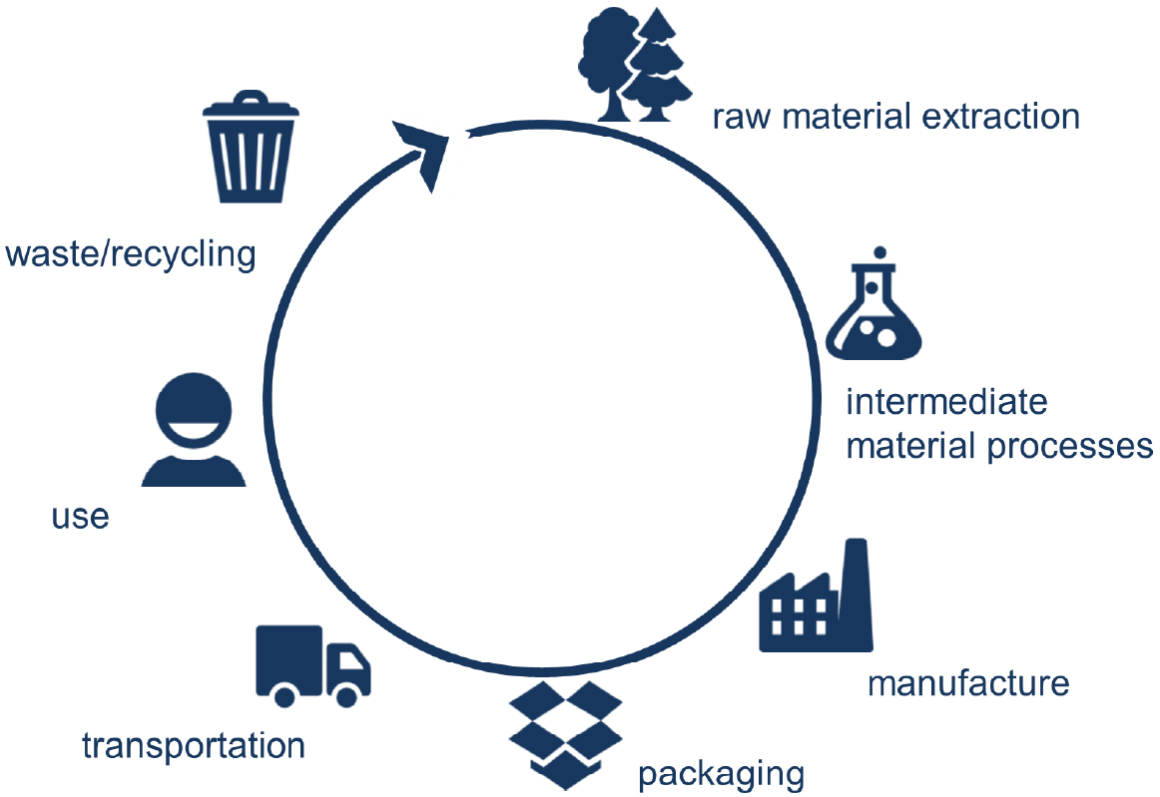
Things to Consider



Use (part 1)

- What are the impacts during use?
- What are the exposure pathways?
- Has the method of application changed exposure duration or intensity?

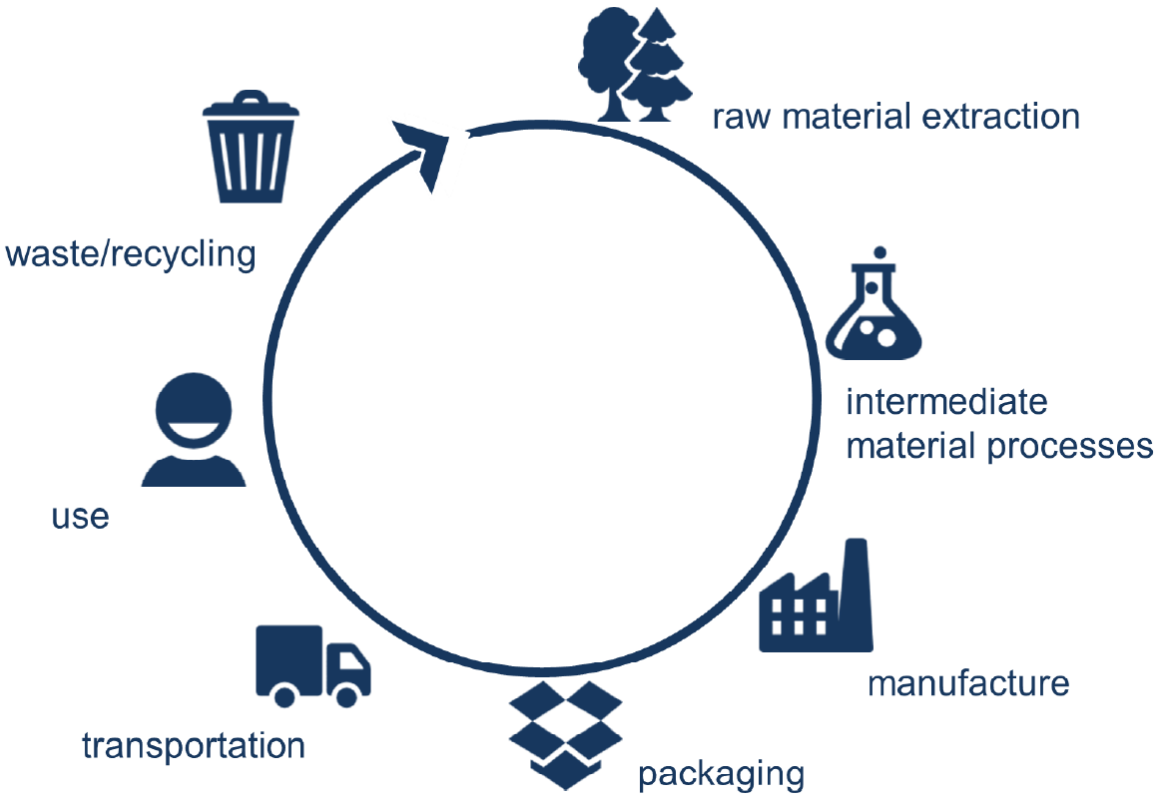
Things to Consider



Use (part 2)

- Has the quantity of product required changed?
- Have new routes of exposure been introduced by an alternative?

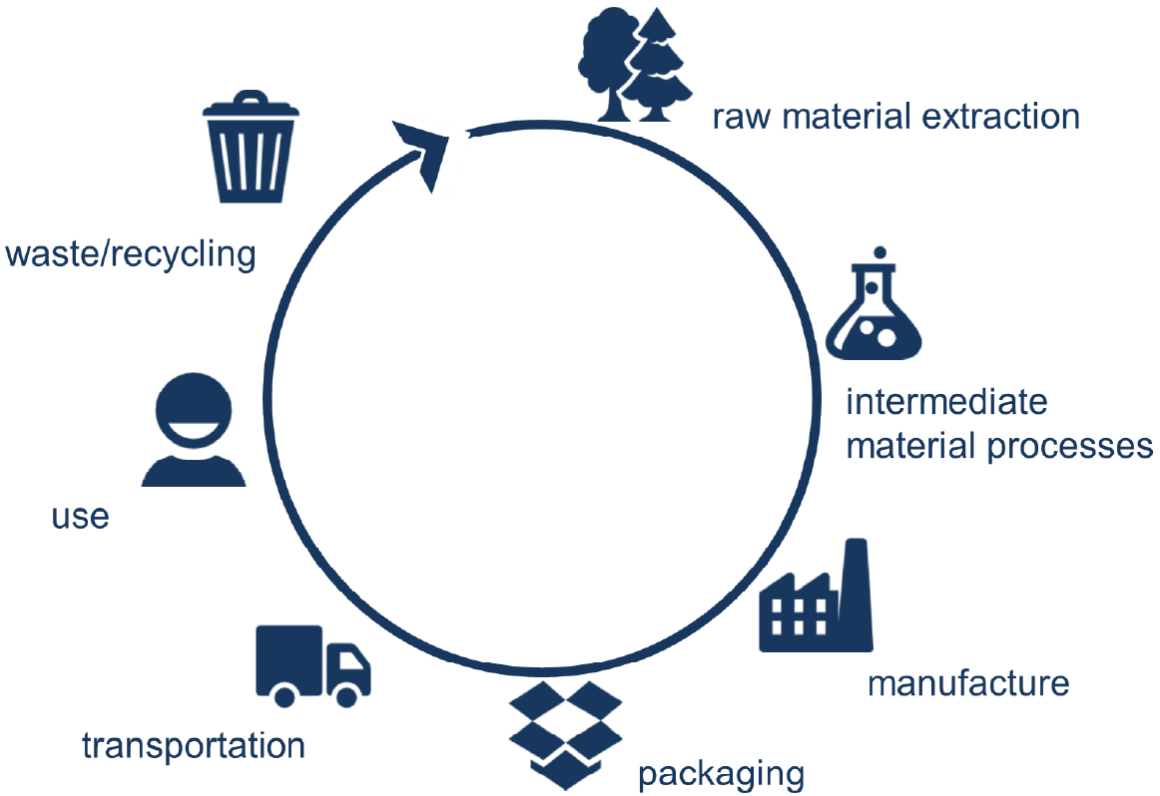
Things to Consider



Operation and Maintenance

- What kinds of chemicals or products are necessary for maintenance?
- How much energy is used to operate or maintain?
- Is there a difference in the reliability or durability of the alternatives?

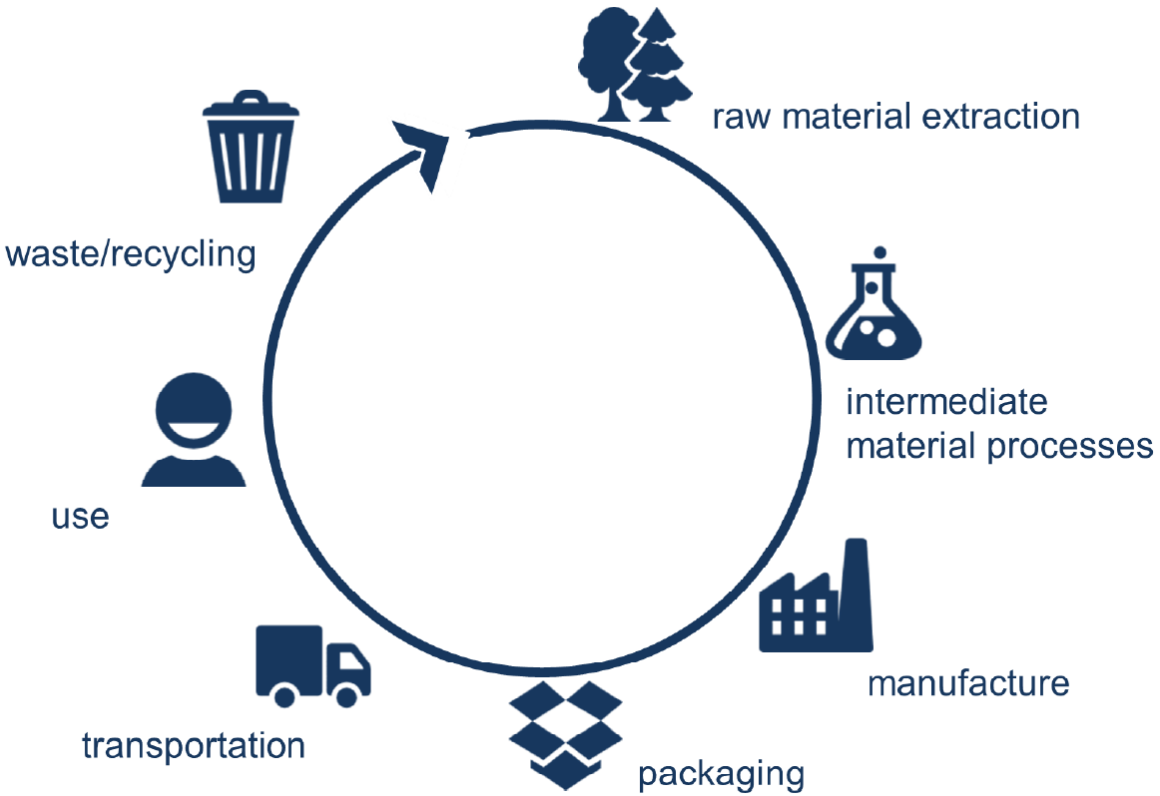
Things to Consider



Waste Generation and Management (part 1)

- How much waste is generated?
- Is hazardous waste generated?
- Are there releases required to be reported under the Toxic Release Inventory program?

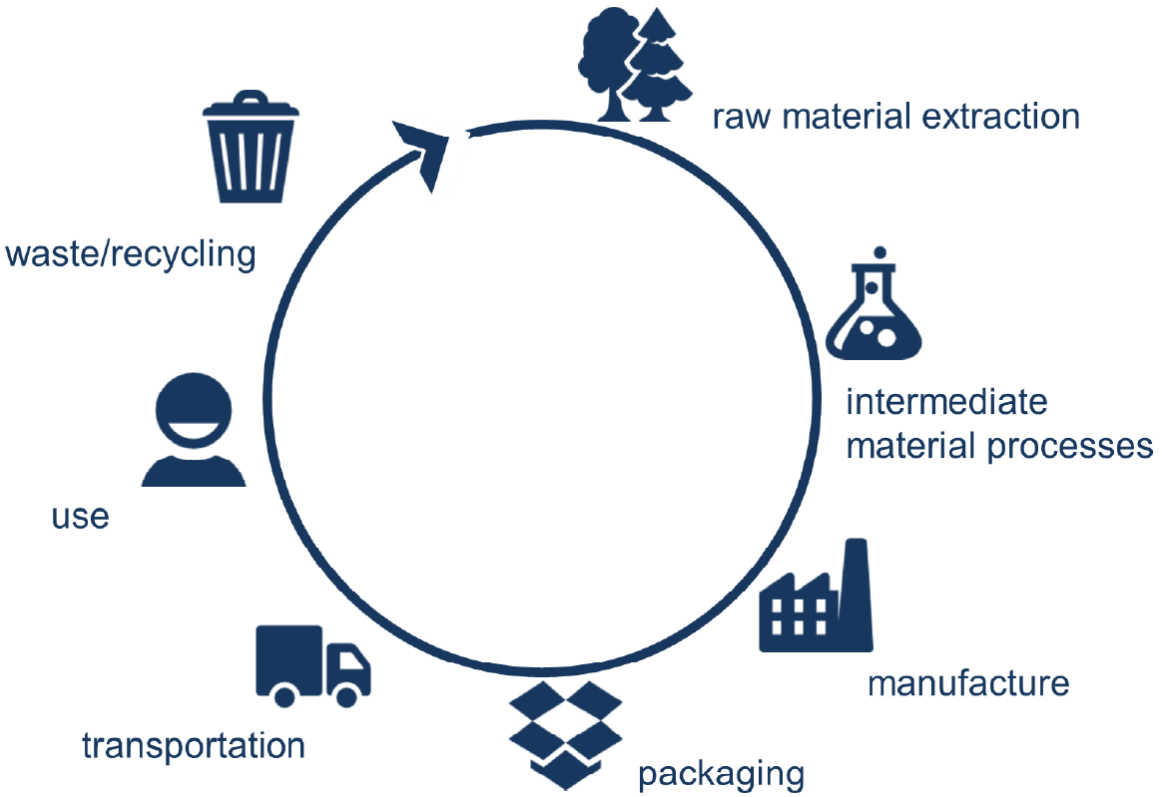
Things to Consider



Waste Generation and Management (part 2)

- Is there any special handling required?
- Does the responsible entity mitigate waste generation impacts by participating in extended producer responsibility programs?

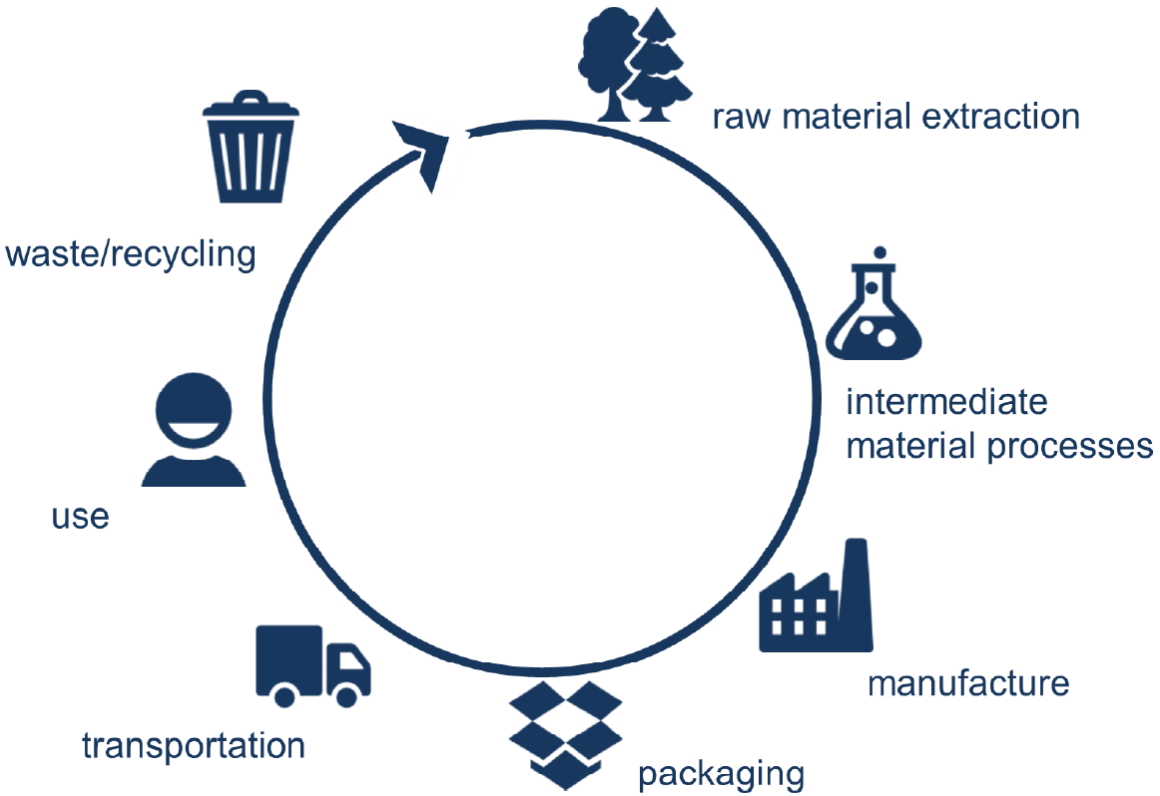
Things to Consider



Reuse and Recycling

- Will there be a change in how the product can be reused or recycled?
- Is there a potential for exposure to a Chemical of Concern during reuse or recycling?

Things to Consider



End-of-life Disposal

- How is the product used and where does it end after its use, i.e., landfill, POTW, air, soil?
- What is the potential for releases of Chemicals of Concern to air or water bodies from the identified disposal?
- Is the Priority Product or the alternative a hazardous waste at end-of-life?

Appendix 3-2 Checklists for Identification of Relevant Factors

TABLE 3-2A EXAMPLE CHECKLIST FOR IDENTIFICATION OF RELEVANT LIFE CYCLE SEGMENTS

Life cycle segments to be considered – Changes between the Priority Product and the alternative being considered	Likely to be a relevant life segment that requires further assessment? Yes/No/Unknown	If "no," reason why the certain life segment not relevant.
Could the alternative change raw materials extraction and processing (e.g., process involved, energy used, resources consumed, and discharge to air/water/soil)?		
Could the alternative change intermediate materials production processes (e.g., process involved, raw materials used, energy used, resources consumed, and discharge to air/water/soil)?		

From AA Guide p175

Table 7-3 Matrix for Simplified Evaluation of Alternatives at Various Life Cycle Stages											
	Raw material extraction	Intermediate material processes	Manufacture	Packaging	Transportation	Distribution	Use	Operation and Maintenance	Waste generation and management	Reuse and recycling	EOL disposal
Impact: Human Health											
Priority Product	L	H	H				H				H
Alternative A	H	H	M				L				L
Alternative B	L		M				M				M
Alternative C	M	H	H				H				M
Alternative D	L	L	L				M				L
Alternative E	L	L	M				M				M
Impact: Air Quality											
Priority Product	H	M	L				L				L
Alternative A	H	H	M				L				L
Alternative B	H		H				H				H
Alternative C	M	M	M				H				H
Alternative D	L	L	L				L				L
Alternative E	L	L	M				M				M

From AA Guide p87

LCA Resources

Some LCI Data Sources

- Process:
  - Ecoinvent (www.ecoinvent.org)
  - US LCI (www.nrel.gov/lci/)
  - Open LCA (http://www.openlca.org/)
  - GREET Model (https://greet.es.anl.gov/)
  - BEES 3.0 (https://www.nist.gov/services-resources/software/bees)
  - CLiCC LCI (http://clicc.net)
- Economic input-output
  - CEDA (https://ghgprotocol.org/Third-Party-Databases/CEDA)
  - Carnegie Mellon (www.eiolca.net/)

Some LCA Software

- Gabi (http://www.gabi-software.com/america/index/)
- SimaPro (https://simapro.com/)
- Quantis Suite (https://quantis-intl.com/)
- CMLCA (http://www.cmlca.eu/)
- openLCA (http://www.openlca.org/)
- Umberto (https://www.ifu.com/en/umberto/?)

CLiCC LCI Example

Cradle-to-Gate Life Cycle Inventory

Methodology | Export All Data

Estimated total inputs and emissions from producing **1 kg** of Dichloromethane:

Name	Amount	Unit	Type	Compartment
1,4-Butanediol	1.25E-10	kg	Emission	Water
1-Pentanol	7.26E-12	kg	Emission	Water
1-Pentene	5.49E-12	kg	Emission	Water
2,2,4-Trimethyl Pentane	1.35E-23	kg	Emission	Air
2,4-D	2.37E-08	kg	Emission	Soil
2-Aminopropanol	7.34E-12	kg	Emission	Water
2-Methyl Pentane	2.94E-09	kg	Emission	Air
2-Methyl-1-Propanol	1.87E-11	kg	Emission	Water
2-Methyl-2-Butene	8.75E-13	kg	Emission	Water
2-Nitrobenzoic Acid	5.25E-12	kg	Emission	Air
2-Propanol	1.08E-10	kg	Emission	Water
4-Methyl-2-Pentanone	3.40E-10	kg	Emission	Water
Acenaphthene	1.76E-11	kg	Emission	Water
Acenaphthylene	1.10E-12	kg	Emis	

Sample of Emission

Sample of Input

Aluminium, 24% In Bauxite, 11% In Crude Ore, In Ground	5.79E-07	kg	Input	Natural Resources
Aluminium, In Ground	3.78E-03	kg	Input	Natural Resources
Anhydrite, In Ground	1.44E-08	kg	Input	Natural Resources
Argon-40	5.78E-05	kg	Input	Natural Resources
Barite, 15% In Crude Ore, In Ground	3.76E-04	kg	Input	Natural Resources
Basalt, In Ground	6.96E-04	kg	Input	Natural Resources
Borax, In Ground	7.21E-07	kg	Input	Natural Resources
Bromine, 0.23% In Water	6.66E-08	kg	Input	Natural Resources
Cadmium, 0.30% In Sulfide, Cd 0.18%, Pb, Zn, Ag, In, In Ground	1.81E-05	kg	Input	Natural Resources
Calcite, In Ground	2.14E-01	kg	Input	Natural Resources
Carbon Dioxide, In Air	7.85E-02	kg	Input	Natural Resources
Carbon, Organic, In Soil Or Biomass Stock	4.69E-05	kg	Input	Natural Resources
Carnallite	8.09E-07	kg	Input	Natural Resources

Some LCIA Methods

METHODS	Acidification	Climate change	Resource depletion	Ecotoxicity	Energy Use	Eutrophication	Human toxicity	Ionising Radiation	Land use	Odour	Ozone layer depletion	Particulate matter/ Respiratory inorganics	Photochemical oxidation
CML (baseline)	✓	✓	✓	✓	-	✓	✓	-	-	-	✓	-	✓
CML (non baseline)	✓	✓	✓	✓	-	✓	✓	✓	✓	✓	✓	-	✓
Cumulative Energy Demand	-	-	-	-	✓	-	-	-	-	-	-	-	-
eco-indicator 99 (E)	✓	✓	✓	✓	-	✓	✓	✓	✓	-	✓	✓	-
eco-indicator 99 (H)	✓	✓	✓	✓	-	✓	✓	✓	✓	-	✓	✓	-
eco-indicator 99 (I)	✓	✓	✓	✓	-	✓	✓	✓	✓	-	✓	✓	-
Eco-Scarcity 2006	-	-	✓	-	-	-	-	-	-	-	-	-	-
ILCD 2011, endpoint	✓	✓	-	-	-	✓	✓	✓	✓	-	✓	✓	✓
ILCD 2011, midpoint	✓	✓	✓	✓	-	✓	✓	✓	✓	-	✓	✓	✓
ReCiPe Endpoint (E)	✓	✓	✓	✓	-	✓	✓	✓	✓	-	✓	✓	✓
ReCiPe Endpoint (H)	✓	✓	✓	✓	-	✓	✓	✓	✓	-	✓	✓	✓
ReCiPe Endpoint (I)	✓	✓	✓	✓	-	✓	✓	✓	✓	-	✓	✓	✓
ReCiPe Midpoint (E)	✓	✓	✓	✓	-	✓	✓	✓	✓	-	✓	✓	✓
ReCiPe Midpoint (H)	✓	✓	✓	✓	-	✓	✓	✓	✓	-	✓	✓	✓
ReCiPe Midpoint (I)	✓	✓	✓	✓	-	✓	✓	✓	✓	-	✓	✓	✓
TRACI 2.1	✓	✓	✓	✓	-	✓	✓	-	-	-	✓	✓	✓
USEtox	-	-	-	✓	-	-	✓	-	-	-	-	-	-

Table 1: Availability of impact categories per method. ✓ represents that the impact category is contained in the correspondent method and - that not.

GreenDelta, LCIA methods, 2015.

LCA Limitations

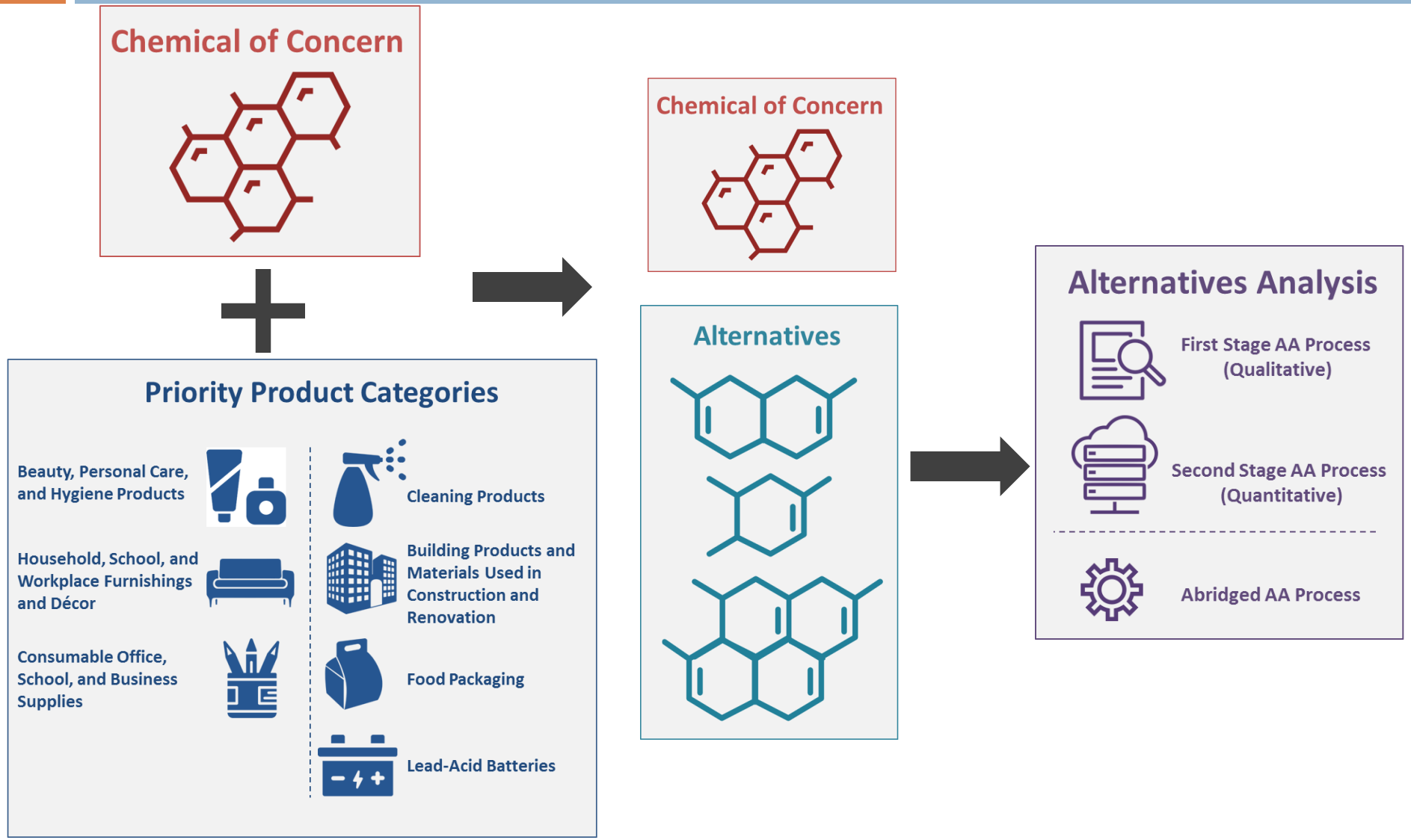
Limitations of LCA approach to AA

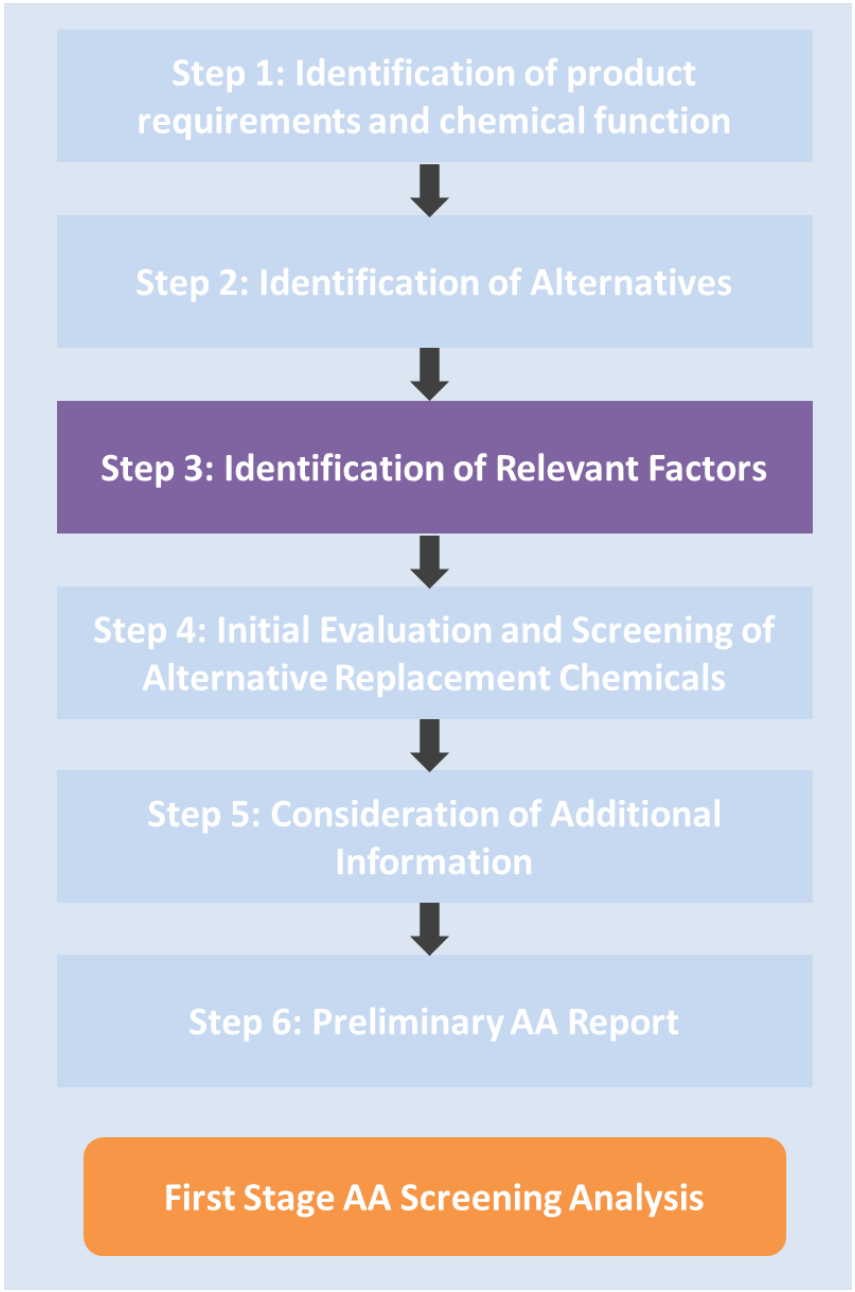
- A full LCA study is costly and time-consuming;
- Data gaps in life cycle inventory of chemicals;
- Data gaps in characterization factors of chemicals;
- LCA alone does not meet all of the requirements in AA;
- What else?

EXPOSURE AND RISK ASSESSMENT IN SUPPORT OF ALTERNATIVES ANALYSIS

Dr. Arturo Keller (Aug 9th, 3:30pm-4:00pm)

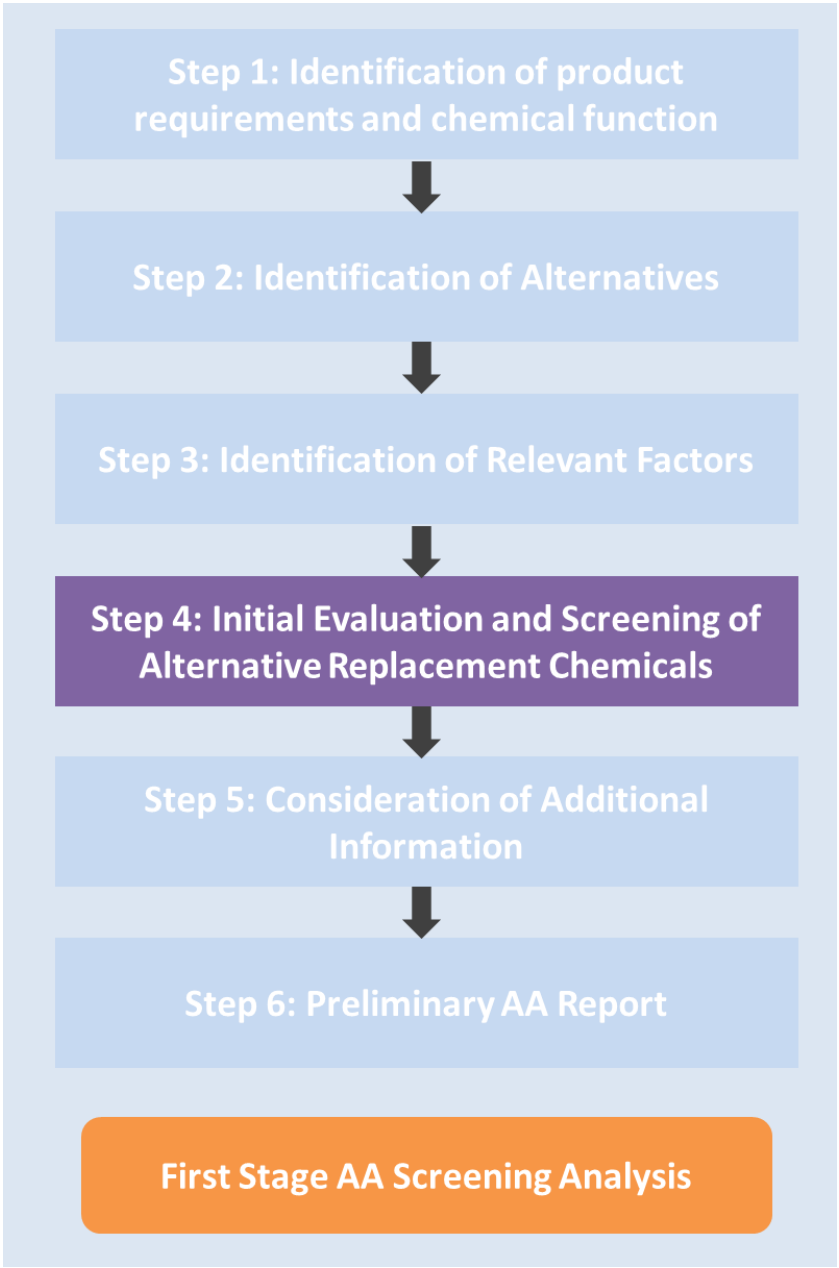
AA Simple Diagram





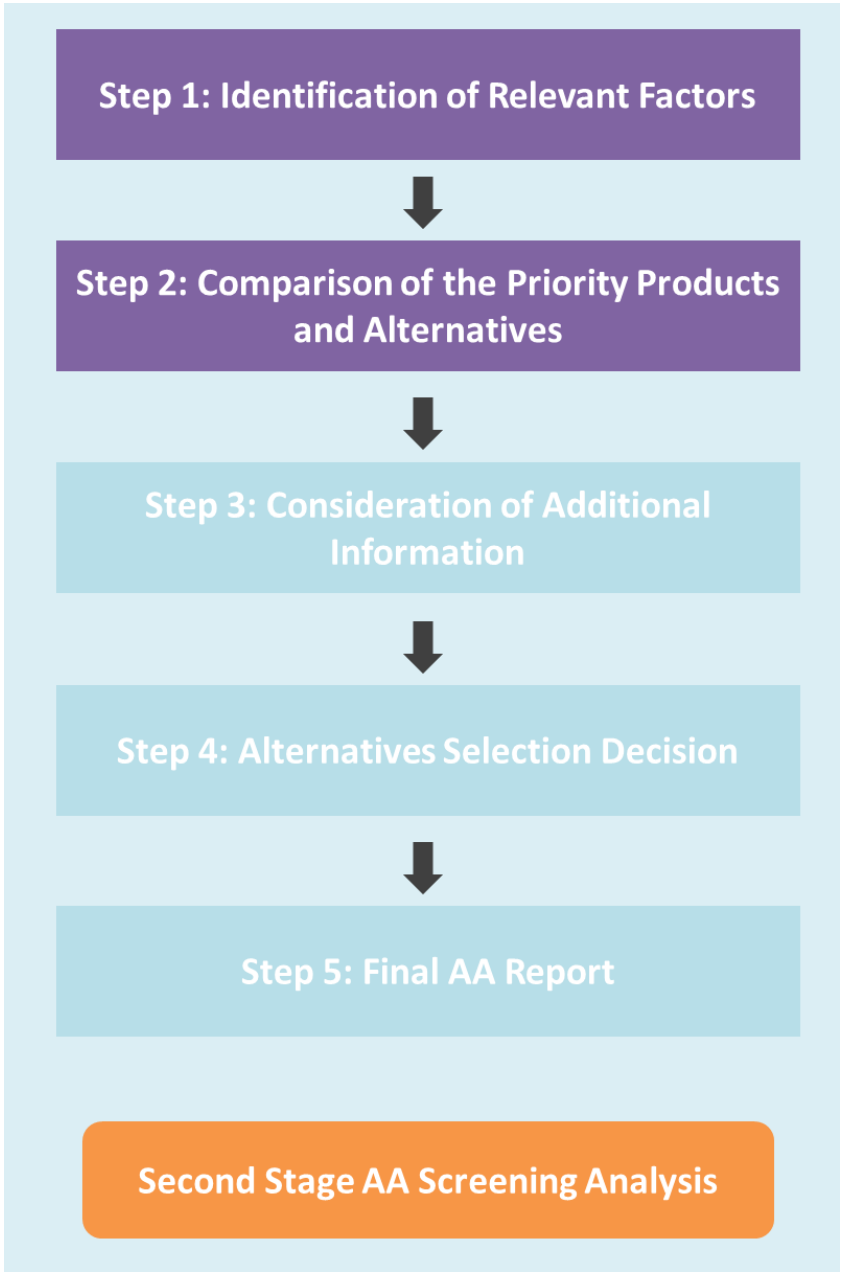
RA Knowledge

- Exposure Pathways



RA Knowledge

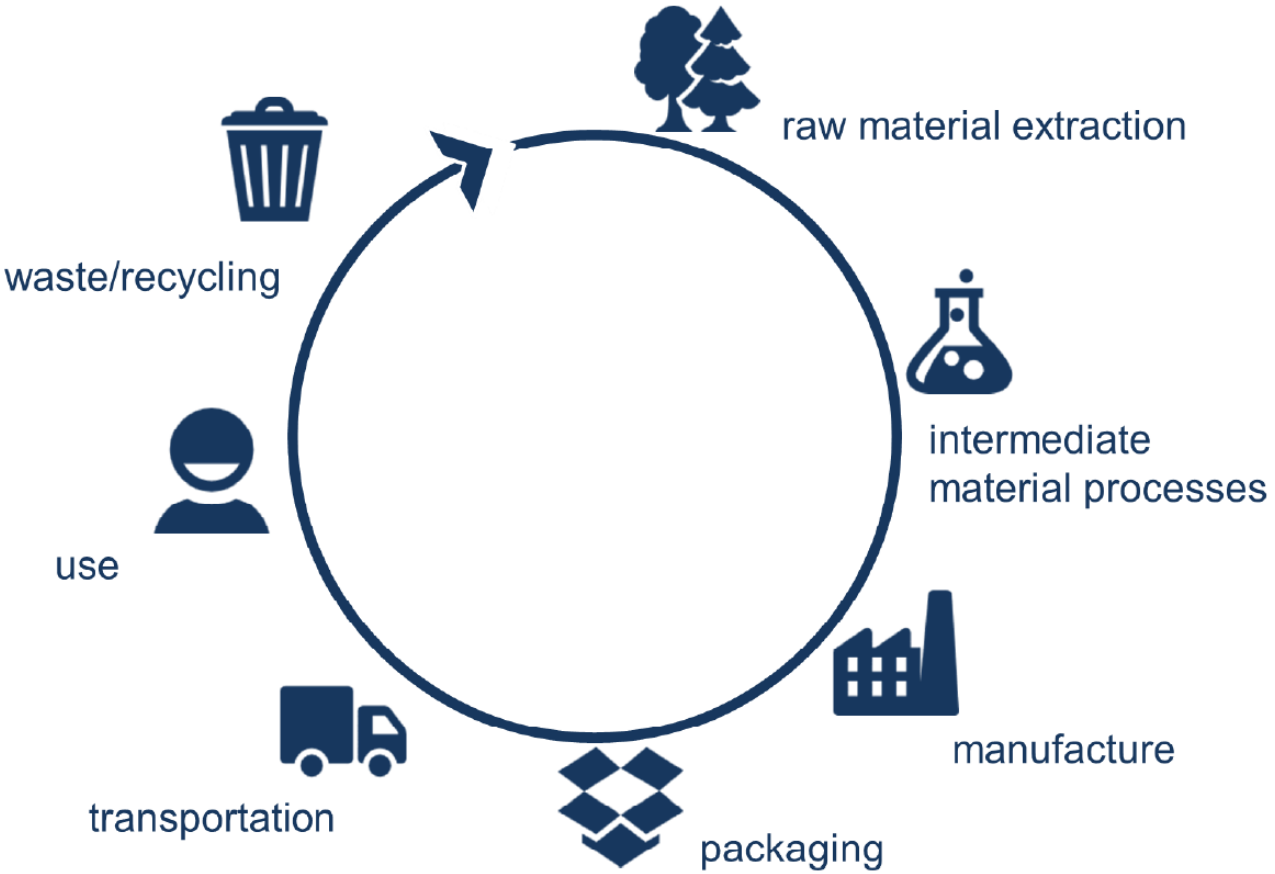
- **Toxicity**
- **Environmental Fate**



RA Knowledge

- Toxicity Assessment
- Exposure Assessment
- Risk Characterization

Toxicity for Emissions Across All Life Cycle Stages



Jordan Chamberlain, Kristen Magnuson, Carolin Meier , Yu Yu, Arturo Keller, Incorporating life cycle screening into Alternatives Analysis.

Comparing Alternatives

- Toxicity considerations
  - Modes of action
  - Acute vs. chronic
  - Ecological risk
- Exposure considerations
  - Release
  - Persistence
  - Routes

Toxicity Considerations

- Carcinogenic toxicity:
  - Are one or more of the alternative chemicals carcinogenic?
  - How well established is the carcinogenicity?
    - Established vs. Preliminary results
    - Consumer perception

Classification of Carcinogens (IARC)

Group	Classification	Agents	Definition
1	Carcinogenic to humans	120	Sufficient evidence in humans, or very strong evidence in animals
2A	Probably carcinogenic to humans	82	Limited evidence in humans, sufficient in animals
2B	Possibly carcinogenic to humans	302	Limited evidence in humans, less than sufficient in animals
3	Not classifiable as to its carcinogenicity to humans	501	Inadequate evidence in humans and inadequate or less than sufficient in animals
4	Probably not carcinogenic to humans	1	Evidence suggesting lack of carcinogenicity

IARC – International Agency for Research on Cancer

https://monographs.iarc.fr/wp-content/uploads/2018/06/CurrentPreamble.pdf

Toxicity Considerations

- Non-carcinogenic toxicity
  - Modes of injury
    - Relevance to route of exposure
      - E.g. toxic effect = skin sensitivity
      - Inhalable? Ingestible?
  - Thresholds
    - RfD
    - NOAEL vs LOAEL
    - Endocrine disruption
    - Skin sensitivity

Toxicity Considerations

- Acute vs. chronic
  - Severity of acute risk
  - Chronic risks may not be observed until large liability exists
  - Consumer behavior
    - Personal protective equipment

Toxicity Considerations

- Methylene chloride
  - Classification: 2B; probable human carcinogen. Basis for classification
    - Based on inadequate human data and sufficient evidence of carcinogenicity in animals
  - oral cancer slope factor = 7.5 x 10-3 (mg/kg/d)-1
- Reference Dose (RfD) = 0.06 mg/kg-d
  - based on liver toxicity in rats
- Acute toxicity: anesthetic effects, nausea and drunkenness

- Benzyl alcohol
  - Carcinogenicity: not classified
  - Acute Ingestion: LD50 (rat) 1230 mg/kg
  - irritating to the skin at levels 3% or greater
  - rats given oral doses of 50, 100, 200, 400, and 800 mg/kg for 13 weeks
    - high dose produced clinical signs indicative of neurotoxicity including staggering, respiratory difficulty, and lethargy

https://pubchem.ncbi.nlm.nih.gov

Toxicity Considerations

- Methylene chloride
  - Daphnia magna
    - ChV = 12.0 mg/L
  - Fish
    - ChV = 24.8 mg/L
    - LC50 fathead minnow = 193 mg/L for 96 hr
  - Green algae
    - EC50 (4 day) = 84.4 mg/L
    - CHv = 19.3 mg/L
  - Earthworm ChV = 173.0 mg/kg
- Benzyl alcohol
  - Daphnia magna
    - Lc50 = 18.3 mg/l
    - ChV = 24.1 mg/L
  - Fish
    - ChV = 53.1 mg/l
    - LC50 fathead minnow = 460 mg/L for 96 hr
  - Green algae
    - CHv = 35.5 mg/L

Exposure Considerations

- **Adverse impacts** of potential exposure are influenced by
  - **Frequency**
  - **Extent** (number of **exposure pathways**)
  - **Level** (**concentration** of the Chemical of Concern or replacement chemical)
  - **Duration** (amount of time)

Exposure Considerations

- Factors to consider
  - Differences in use/release amounts due to
    - Effectiveness for a given function
    - Chemical properties
      - Volatility
      - Solubility
      - Bioaccumulation (octanol/water partitioning)
      - Reactivity

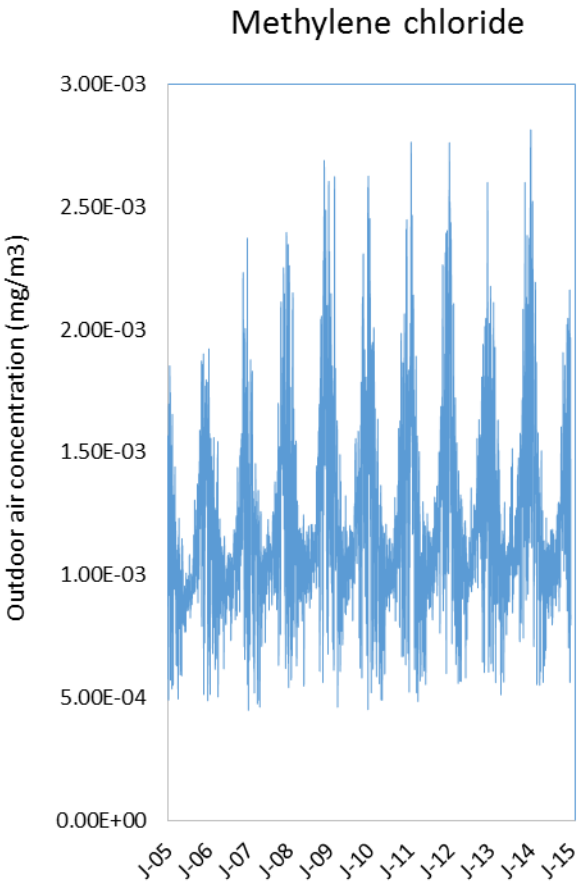
Exposure Considerations

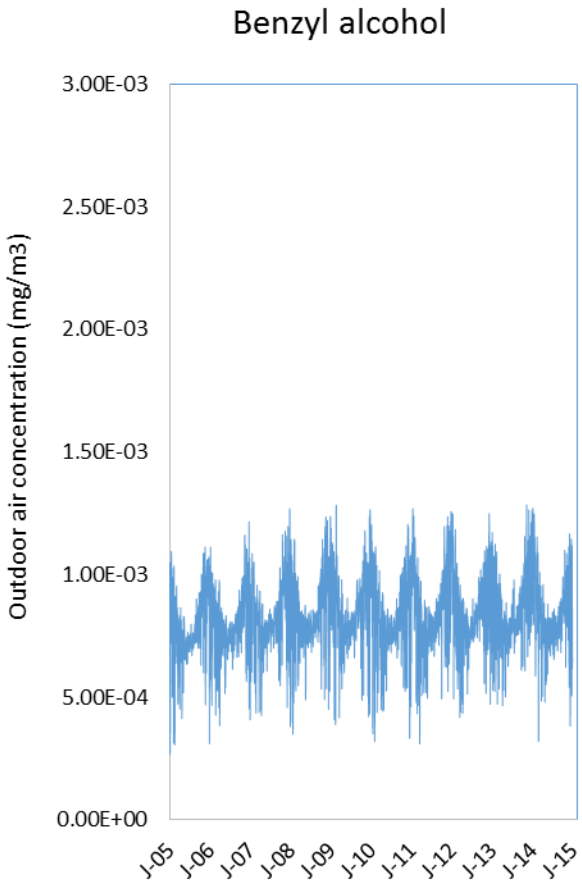
- Methylene chloride
  - VP = 4.70E+04 Pa
  - Sol = 1.30E+04 mg/L
  - Kow = 1.78E+01
  - Half-life:
    - Air = 1.81E+03 hr
    - Water = 9.00E+02 hr
- Benzyl alcohol
  - VP = 1.25E+01 pa
  - Sol = 4.29E+04 mg/L
  - Kow = 1.26E+01
  - Half-life:
    - Air = 1.12E+01 hr
    - Water = 3.60E+02 hr

Fate & Transport

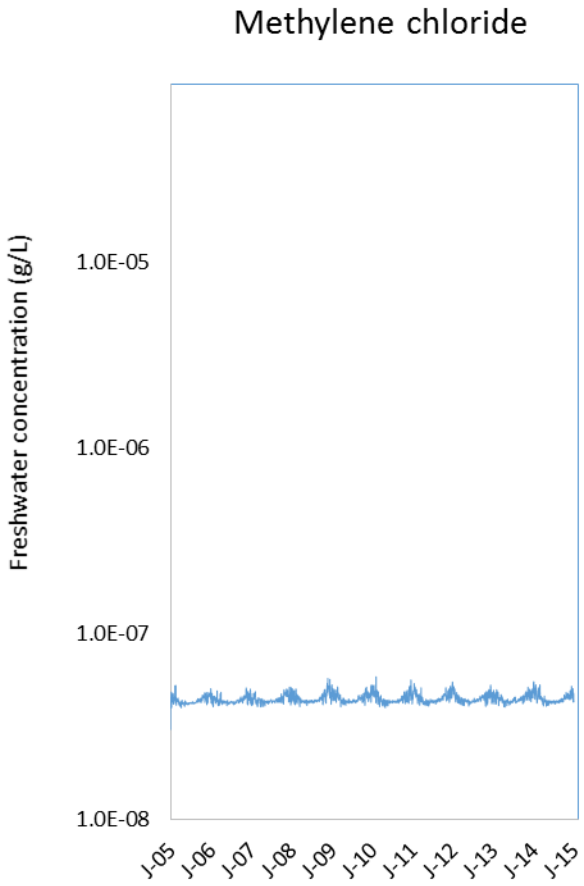
- Dominant pathways
  - How much are they influenced by change in mode of release?
  - Where will the majority of the mass of chemical released end up?
  - Differences in persistence?
  - Different media contaminated?

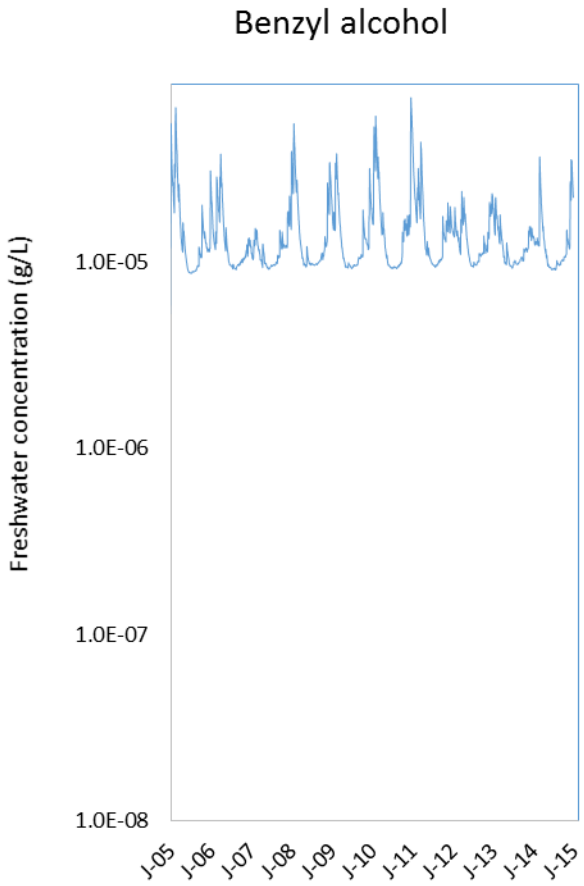
Predicted Concentrations - Outdoor Air





Predicted Concentrations - Freshwater





Indoor Air

Modelling Indoor Air Quality

Use a material balance "box model" to get indoor concentration

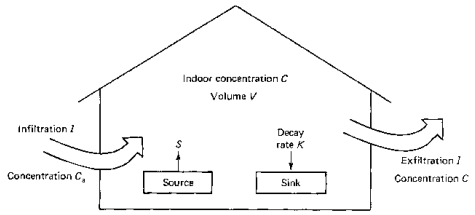


Figure 7.35 Box model for indoor air pollution.

accumulation rate = input rate +sources – output rate – decay

$$V\frac{dC}{dt} = S + C_a IV - CIV - KCV$$

C = indoor concentration (mg/m^3)
V = volume of conditioned space in building (m^3/air change)
I = Q/V = ach = infiltration rate
S = pollutant source strength (mg/hr)
C_a = ambient (=outside) concentration of pollutant (mg/m^3)
K = decay rate or reaction rate of pollutant (hr^{-1})

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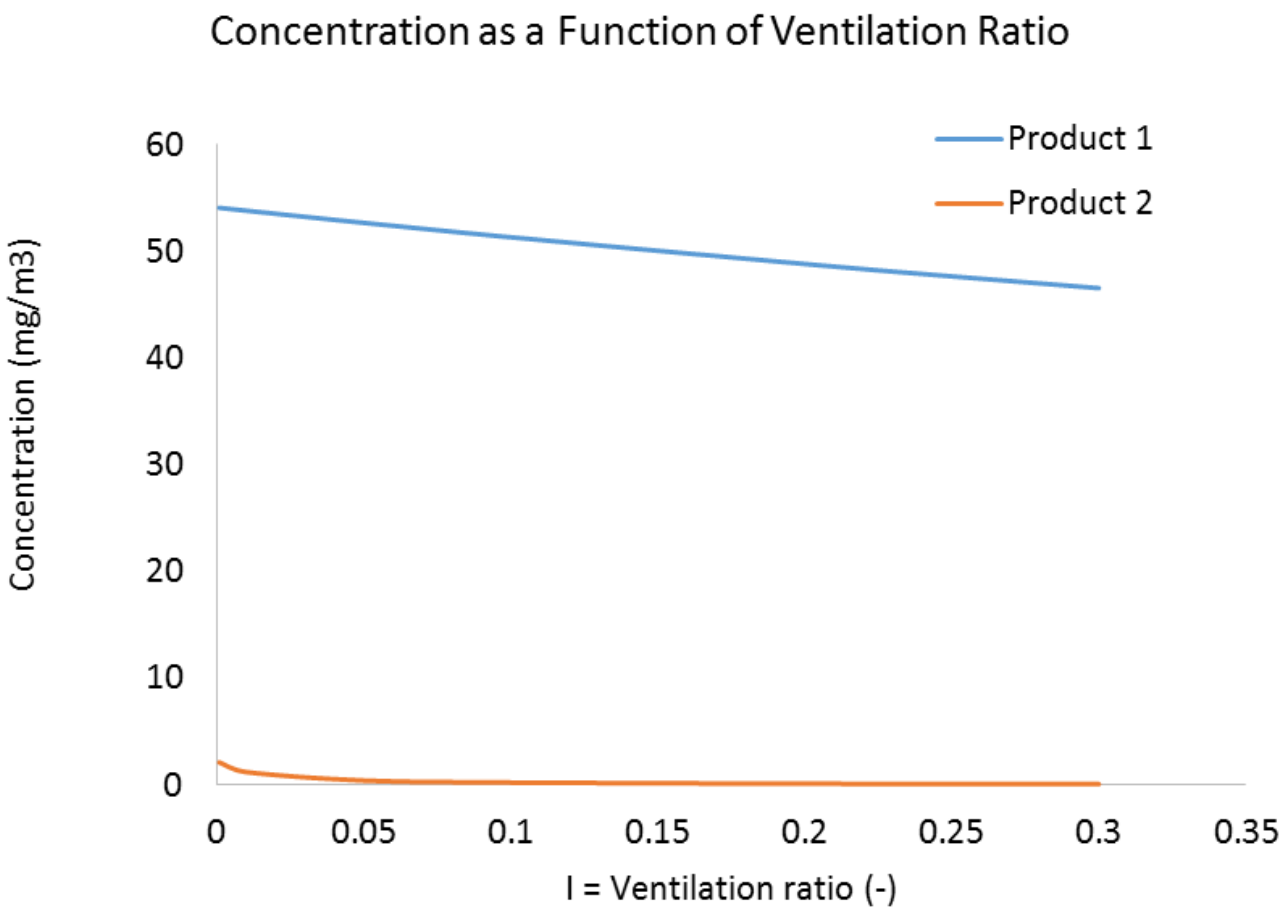
- At steady state,

$$\frac{dC}{dt} = 0$$

- $$C = \frac{S + C_a IV}{IV + kV}$$
- S is direct function of vapor pressure

Predicted Concentrations - Indoor Air



Exposure Assessment

- "Exposure assessment evaluates whether alternatives have **the same, higher, or less exposure level** than the Chemical of Concern"
- Need to take into consideration differences in toxicity, in addition to exposure level

Exposure Assessment

- Differences in exposure frequency or duration
  - Higher functionality may require less frequent application
  - Time to apply the product is faster
  - Easier application leads to less exposure
  - New methods of application reduce exposure

Relevant Exposure Factors

Chemical of Concern

Potential Chemical Alternatives

Used in the same relative **amounts**?

Used in the same **manner**?

At what point during the **life cycle,** could human populations or ecological receptors be exposed to the potential **releases**?

What are the **use patterns**?

What are the potential **types of use** and **end-of-life** exposure scenarios?

What are the expected differences regarding **exposure frequency, extent, level, duration, and routes**?

Could **physicochemical properties** substantively affect exposure pathways?

Will any engineering or administrative controls be used?

What are the differences in how the product contains chemical?

Modified from AA Guide p39

Key Points

- Exposure & risk assessment can be used as part of alternatives analysis
- Toxicity information may not be fully available
  - May need to consider other factors
- Exposure can differ significantly due to:
  - Chemical properties
  - Changes in amount released and release pathways
  - Differences in persistence
  - Differences in exposure factors

QUESTION & ANSWER SESSION

Dr. Sangwon Suh & Dr. Arturo Keller